

# Local lattice disorder in the geometrically-frustrated spin glass pyrochlore $\text{Y}_2\text{Mo}_2\text{O}_7$

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## Abstract

The geometrically-frustrated spin glass  $\text{Y}_2\text{Mo}_2\text{O}_7$  has been considered widely to be crystallographically ordered with a unique nearest neighbor magnetic exchange interaction,  $J$ . To test this assertion, we present x-ray-absorption fine-structure results for the Mo and Y  $K$  edges as a function of temperature and compare them to results from a well-ordered pyrochlore,  $\text{Ti}_2\text{Mn}_2\text{O}_7$ . We find that the Mo-Mo pair distances are significantly disordered at approximately right angles to the Y-Mo pairs. These results strongly suggest that lattice disorder nucleates the spin-glass phase in this material.

Materials with magnetic ions that reside on the corners of triangles or tetrahedra and have a nearest-neighbor antiferromagnetic interaction  $J$  potentially display phenomena known broadly as *geometrical frustration*.<sup>1</sup> Such symmetries preclude a simple two-sublattice Néel ordering, as it is not possible to satisfy all near-neighbor antiferromagnetic interactions. Materials that exhibit frustration can still undergo a magnetic transition whereby spins freeze into a lattice without long-range order, that is, they form a spin glass (SG). Theoretical calculations have long asserted that a SG transition is only possible when both frustration (potentially induced by lattice disorder) and a distribution of effective  $J$ 's exists.<sup>2</sup> Many earlier experimental studies bear this assertion out.<sup>3</sup> Recently, there has been great interest in some SG materials that apparently contradict this assertion.<sup>1</sup> Such systems include the  $\text{Gd}_3\text{Ga}_5\text{O}_{12}$  (GGG)<sup>4</sup> and some pyrochlores such as  $\text{Y}_2\text{Mo}_2\text{O}_7$ .<sup>5-10</sup> In the case of GGG, some off-stoichiometry is known to exist, but is likely too little to explain the SG transition using conventional methods.  $\text{Y}_2\text{Mo}_2\text{O}_7$ , on the other hand, is apparently pure, stoichiometric, and crystallographically well ordered.<sup>5</sup> Consequently, it has been studied with a wide range of techniques. This system displays strong indications of a SG transition at  $T_g=22.5$  K, including irreversible behavior in the bulk magnetic susceptibility<sup>6,7</sup> and a rapid slowing down and freezing of the magnetic moments with no long-range order down to  $\sim 0.1 T_g$  from neutron scattering and muon spin rotation/relaxation ( $\mu\text{SR}$ ) data.<sup>8,9</sup> However, some magnetic properties are anomalous when compared to conventional SG materials.<sup>8,10</sup> Such properties seem to point the way towards some form of new mechanism for SG formation.

Frustration arises in the Mo sublattice of  $\text{Y}_2\text{Mo}_2\text{O}_7$  because the Mo atoms occupy a corner-shared tetrahedral network, making this system a three dimensional analog of the kagomé lattice of a corner-shared triangular network. Although not generally recognized,  $\text{Y}_2\text{Mo}_2\text{O}_7$  has a substantially enhanced displacement parameter for the transition-metal site of  $\langle u^2 \rangle \approx 0.0145 \text{ \AA}^2$  at room temperature<sup>5</sup> (compare to  $0.0075 \text{ \AA}^2$  for the Mn site in the well-ordered pyrochlore  $\text{Tl}_2\text{Mn}_2\text{O}_7$ <sup>11</sup>). Such a large displacement parameter could either be due to an unusually low Debye temperature (i.e. large dynamic displacements due to thermal phonons) for the Mo site, or to static (positional) displacements that are not described well by the standard Rietveld refinement. These facts lead us to search for pair-distance disorder in  $\text{Y}_2\text{Mo}_2\text{O}_7$  using the x-ray-absorption fine-structure (XAFS) technique as a local probe of the Y and Mo environments. Using information about both these environments and comparing to data on  $\text{Tl}_2\text{Mn}_2\text{O}_7$ , we show below that the Mo tetrahedra are, in fact, disordered from their average, ideal structures. Furthermore, the magnitude of this disorder is roughly consistent with the SG transition temperature  $T_g$  and mean-field theory (MFT).<sup>12</sup>

The polycrystalline sample is the same sample used in Ref. 9, and was prepared and characterized in a similar manner to that reported previously.<sup>5-8</sup> In particular, field-cooled and zero field-cooled magnetization measurements were performed which displayed the signature irreversible behavior and a  $T_g = 22.5$  K, indistinguishable from that reported previously.<sup>7</sup> A neutron powder diffraction study indicates the deviation from nominal oxygen stoichiometry is less than 1%,<sup>9</sup> and is consistent with previous studies in all respects, including the  $\langle u^2 \rangle$  parameters.<sup>5</sup> Before collecting x-ray absorption data, the sample was ground under acetone, sifted through a  $30 \mu\text{m}$  sieve, and brushed onto scotch tape. Strips of tape were stacked such that the Mo  $K$  (20 keV) and Y  $K$  (17 keV) absorption steps were about one absorption length. The samples were loaded into a LHe flow cryostat, and absorption spectra were collected between 15-300 K on BL 4-1 at the Stanford Synchrotron Radiation Laboratory

(SSRL) using Si(220) monochromator crystals.

The XAFS technique involves measuring and analyzing the absorption spectrum just above an absorption edge. Oscillations occur when the outgoing photoelectron (p.e.) is partially backscattered by neighboring atoms, interfering with the outgoing component. The interference depends on the p.e. wave vector  $k$ , and on the pair-distance distribution of the various atomic shells. An oscillatory function,  $\chi(k)$ , is extracted and the Fourier transform (FT) of  $\chi(k)$  gives peaks in  $r$ -space that correspond to various coordination shells. FT's are not exactly radial-distribution functions, however, and fits need to be performed to extract numerical structural information. These fits provide the pair distance  $R$  from the absorbing atomic species to a given shell around that atom, the pair-distance distribution variance  $\sigma^2$  and, in some cases, the skewness of the distribution, which we report in terms of cumulants.<sup>13</sup>

All data reduction and fits in this paper utilize the standard procedures in Ref. 14–16. In particular, we fit the FT of  $k^3\chi(k)$  to backscattering and phase functions calculated by FEFF7.<sup>17</sup> The following results focus on single-scattering paths, although multiple scattering is included in the analysis. Each backscattering species was allowed to have a different p.e. threshold energy. Errors reported for the XAFS fit parameters  $R$  and  $\sigma^2$  are based on the reproducibility of the fits for each of the three scans taken at each temperature. Absolute errors for these parameters are typically much larger,<sup>15</sup> about 10% for nearest neighbors and roughly 20% for further neighbors in  $\sigma^2$ , and about 0.01 Å for nearest neighbors and 0.02 Å for further neighbors  $R$ .

To demonstrate that an ordered pyrochlore can accurately be measured using XAFS, we chose to measure the “colossal” magnetoresistance material  $\text{Tl}_2\text{Mn}_2\text{O}_7$ . These data were partially analyzed earlier.<sup>18</sup> An example of the XAFS data at  $T = 50$  K is presented in Fig. 1. The nominal structure is the same as  $\text{Y}_2\text{Mo}_2\text{O}_7$  with Tl and Mn replacing Y and Mo, respectively. Rietveld refinements<sup>11</sup> show that each Tl site has six O(1) neighbors at 2.43 Å and two O(2)'s at 2.15 Å. The XAFS from these oxygens interfere with each other, reducing their combined amplitude and producing the peak centered at about 2 Å in the FT data. The oxygen coordination for Mn is similar with six O(1)'s at 1.90 Å, but without any further nearest-neighbor oxygens, and therefore the XAFS has a much stronger peak in the FT at  $\sim 1.6$  Å. The next-nearest-neighbor coordination for the Tl and Mn sites are the same, with six Mn and six Tl neighbors at 3.49 Å (a “Tl/Mn” peak at  $\sim 3.3$  Å in Fig. 1). These occupancies are assumed in the fits.

Table I shows the fit results from the Tl  $L_{III}$  and Mn  $K$  edge XAFS of  $\text{Tl}_2\text{Mn}_2\text{O}_7$ . Data were collected from 50–300 K, and no abnormal temperature dependence in either the pair distances or distribution variance was observed. The pair-distance distribution variance  $\sigma^2$  for each pair of atoms is described well by a correlated-Debye model<sup>19</sup> (i.e. phonons) with no appreciable static disorder. The correlated-Debye model has been shown to describe the temperature dependence of  $\sigma^2$  with no additional temperature independent offset (“static”) component for the well-ordered oxide  $\text{CaMnO}_3$ . If an offset is necessary, it is quantitatively equal to extra lattice disorder as in  $\text{La}_{1-x}\text{Ca}_x\text{MnO}_3$ .<sup>20</sup> In any case, rather than show the temperature dependence of  $\sigma^2$  for each shell, we merely list the correlated-Debye temperature  $\Theta_{cD}$  and offset  $\sigma_{\text{stat}}^2$  in Table I.

Figure 2 shows the data and fits for  $\text{Y}_2\text{Mo}_2\text{O}_7$  at  $T = 15$  K. The raw data already strongly indicate some unexpected disorder in the Y/Mo peak. Since these environments are nominally the same, this peak should have nearly the same amplitude for both the Mo

and Y edge data. However, as is seen in Fig. 2, the Mo-Mo/Y peak is only about 25% the size of the Y-Mo/Y peak. Table II summarizes these fits for  $T = 15$  K. Like the fits to the  $\text{Ti}_2\text{Mn}_2\text{O}_7$  data, we find no abnormal atom-pair distances compared to the diffraction results. However, we do measure a large temperature-independent contribution to  $\sigma^2$  in several atom pairs, most significantly in the Mo-Mo pairs. Several atom pairs show a  $\sigma_{\text{stat}}^2$  contribution that is significantly larger than the estimated errors. In particular, the Mo-Mo peak is almost completely washed out by its estimated static variance of  $\sim 0.03 \text{ \AA}^2$ , while the Y-O(1) and Y-Mo/Y pairs also display a modest static component to their variance. Since the Y-Mo pairs also include Mo atoms, we conclude that the primary direction of the large disorder in the Mo-Mo pairs is roughly perpendicular to the Y-Mo pairs and parallel to the Mo-Mo pairs. Notice that, in spite of the large measured disorder, the diffraction results are in rough agreement with these XAFS results: If one assumes the Mo displacements are uncorrelated with each other, one expects the XAFS measured variance in the Mo-Mo pairs to be roughly  $2 \langle u^2 \rangle \approx 0.029 \text{ \AA}^2$ , in agreement with the measured value of  $0.026(5) \text{ \AA}^2$ .

The particularly large magnitude of the Mo-Mo variance  $\sigma^2$  led us to attempt to fit this pair assuming some form of anharmonic distribution. Including a split peak in the fit did not produce satisfactory results. Some improvement to the fit was made by including a significant skewness in the Mo-Mo distribution, with a third-cumulant  $C_3 = -0.080 \pm 0.005 \text{ \AA}^3$ ,<sup>13</sup> which also decreases the fitted  $\sigma_{15\text{K}}^2$  to about  $0.01 \text{ \AA}^2$ . Notice that the total disorder is approximately unchanged in this fit. However, the overall improvement to the fit was not very significant. With any description, however, the conclusion is that the Mo-Mo pairs cannot be completely described by a single harmonic potential.

Table II shows that the Mo-O(1) octahedron remains a tightly bound unit, with a high  $\Theta_{\text{CD}}$  and little static disorder. If the Mo disorder carries the O(1) octahedron with it, then the Y-O(1) pairs must also be disordered. Furthermore, the Y-Mo pair should show some disorder if the Mo-Mo disorder is so large. Indeed, for both these pairs we do measure some excess disorder in  $\sigma_{\text{stat}}^2$ .

Although the disorder in the Mo-Mo pairs is obvious in the XAFS data, at this time we can only speculate why such disorder exists in  $\text{Y}_2\text{Mo}_2\text{O}_7$  and not in  $\text{Ti}_2\text{Mn}_2\text{O}_7$ . One possibility is that a very small ( $\lesssim 1\%$ ) number of oxygen vacancies create enough  $\text{Mo}^{3+}$  ions to precipitate the measured disorder. This situation is very unlikely because we then expect equally strong disorder in the  $\text{MoO}_6$  octahedra, which we do not observe. Similarly, any significant Y/Mo site interchange seems unlikely due to the observed order in the Y environment and the  $\text{MoO}_6$  octahedra, as well as ionic size arguments. Another more intriguing possibility is that the Mn tetrahedra in  $\text{Ti}_2\text{Mn}_2\text{O}_7$  are ordered because of the metallic Ti  $6s$  band and its interaction with the Mn  $3d$  band. This mechanism is not present in  $\text{Y}_2\text{Mo}_2\text{O}_7$ , so the more localized Mo  $4d$  band may allow the disorder to develop. Comparisons to data on the SG  $\text{Tb}_2\text{Mo}_2\text{O}_7$  and the ferromagnet  $\text{Y}_2\text{Mn}_2\text{O}_7$  may help clarify this issue.

The above measurements show that the primary disorder involves only the Mo atoms in a direction that is roughly parallel to local Mo-Mo pairs and perpendicular to Mo-Y pairs. One possible distortion is shown in the inset to Fig. 2(b) by displacing the Mo atom towards or away from the tetrahedron body center. The magnitude of this distortion may vary throughout the solid, creating a distribution of Mo-Mo pair distances and not severely altering the Mo-Y pairs. Displacing the Mo towards a tetrahedron corner will similarly distort the Mo-Mo pairs while having little effect on the Mo-Y environment.

The Mo disorder has a very important implication for understanding the SG behavior of  $\text{Y}_2\text{Mo}_2\text{O}_7$ : the fundamental assertion that a SG transition at finite temperature should not occur without both frustration and disorder in  $J$  now appears to hold for  $\text{Y}_2\text{Mo}_2\text{O}_7$ . It is, however, important to ask whether the measured disorder is enough to explain the magnitude of  $T_g$ . We first define the disorder in  $J$  as  $\sigma_J/J_0$  with a mean magnetic interaction  $J_0$  and a variation in  $J$  of  $\sigma_J^2$ . To estimate the effect of pair-distance disorder, we use the simple Heitler-London result that  $J \propto 1/R$  with a variation  $\sigma_R^2$  in the pair-distance distribution and a mean distance  $R_0$ . This approximation gives  $\sigma_J/J_0 \approx \sigma_R/R_0 \approx 5\%$  for this XAFS measurement. We then compare this value of the disorder due to bond length variations to the disorder in  $J$  estimated from the quantum-mechanical MFT with Ising spins of Sherrington and Southern (SS).<sup>12</sup> Using Eq. 12 in SS with a coordination  $z = 6$ ,  $T_g = 20\text{K}$  and  $S = 2$  for a  $\text{Mo}^{4+}$  ion, we obtain  $\sigma_J = 0.39\text{ meV}$ . Similarly, using Eq. 17 in SS together with the measured Curie-Weiss temperature  $\Theta_{\text{CW}}$  of  $200\text{ K}$ ,<sup>7</sup> we obtain  $J_0 = 1.74\text{ meV}$ . Therefore, according to SS, we expect to find the same ratio  $\sigma_J/J_0$  to be  $\approx 20\text{-}25\%$ .

When comparing the expected disorder of  $20\text{-}25\%$  in the SS theory to that approximated from the pair-distance disorder of  $\sim 5\%$ , it is important to remember that the SS theory uses many approximations, including Ising spins, nearest-neighbor-only interactions and MFT. With these caveats, the fact that SS theory predicts the same order of magnitude of disorder in  $J$  as estimated from the lattice disorder indicates strongly that lattice disorder plays a major role in the SG transition. On the other hand, the measured disorder is still a factor of 5 less than expected from the SS arguments, and so it is very unclear whether  $\text{Y}_2\text{Mo}_2\text{O}_7$  belongs in the class of low-disorder spin glasses such as GGG or not. Therefore it is very important that both Monte Carlo calculations be performed using the measured disorder and that other probes be used to clarify the exact nature of the disorder. Pair-distribution-function analysis of neutron or x-ray diffraction data might be very helpful in this regard once the general parameters of the disorder from the XAFS measurements are included.<sup>21</sup> Such Monte Carlo calculations should clarify if pair-distance disorder (as opposed to substitutional disorder) can explain any of the unconventional properties in  $\text{Y}_2\text{Mo}_2\text{O}_7$ .<sup>8,10</sup>

In summary, we have performed temperature dependent XAFS experiments at both the Y and Mo  $K$  edges on a well characterized sample of  $\text{Y}_2\text{Mo}_2\text{O}_7$ . These measurements indicate a relatively large amount of pair-distance disorder (between  $0.1$  and  $0.2\text{ \AA}$ ) of the Mo atoms exists, roughly perpendicular to the Y-Mo pairs and possibly in the direction of the Mo tetrahedron face centers. In addition, the oxygen octahedron surrounding the Mo site is roughly preserved, while the octahedron surrounding the Y site is distorted. These measurements indicate that lattice disorder does exist in these materials in the form of pair-distance disorder, and therefore the theoretical requirement that disorder in  $J$  exist for a SG transition to occur appears to be met. The degree of disorder is still low when compared to that expected from MFT, underlining the need for a new approach towards understanding low-disorder spin glasses both by better characterization of existing disorder and from theoretical descriptions that include these characterizations.

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# TABLES

TABLE I. Fit results for Tl and Mn edge data on  $\text{Tl}_2\text{Mn}_2\text{O}_7$ .  $S_0^2=1.0$  for the Tl edge fits and 0.92 for the Mn edge fits. Results for  $\sigma^2$  and  $R$  are at  $T=50$  K. See text for a discussion of errors on  $R$  and  $\sigma^2$ . Error estimates for  $\sigma_{\text{stat}}^2$  and  $\Theta_{\text{cD}}$  are based on the covariance matrix from the least-squares fit to  $\sigma^2(T)$ . Superscripts \* and # indicate values constrained to be the same in the fits.

atom pair	$\sigma^2$ ( $\text{\AA}^2$ )	$R$ ( $\text{\AA}$ )	$\Theta_{\text{cD}}$ (K)	$\sigma_{\text{stat}}^2$ ( $\text{\AA}^2$ )
Mn-O(1)	0.0025(1)	1.902(2)	800(70)	0.0001(3)
Mn-Mn	0.0037(1)	3.492(2)*	600(60)	0.0014(4)
Mn-Tl	0.0026(1)	3.492(2)*	275(30)	0.0001(1)
Tl-O(1)	0.0060(1)	2.431(1)	480(30)	0.0008(6)
Tl-O(2)	0.0011(2)	2.146(1)	850(90)	-0.0001(3)
Tl-Tl	0.0023(1)	3.491(1)#	345(10)	-0.0002(2)
Tl-Mn	0.0024(1)	3.491(1)#	230(20)	0.0002(5)

TABLE II. Fit results for Y and Mo edge data on  $\text{Y}_2\text{Mo}_2\text{O}_7$ .  $S_0^2=1.0$  for the Y edge and 0.83 for the Mo edge fits. Results for  $\sigma^2$  and  $R$  are at  $T = 15$  K. Note that  $\sigma^2$ 's and  $R$ 's for Y-Y and Y-Mo were constrained together. Also note that  $\Theta_{\text{cD}}$  was held fixed at 260 K to estimate  $\sigma_{\text{stat}}^2$ , but that no resolvable temperature dependence was observed.

atom pair	$\sigma^2$ ( $\text{\AA}^2$ )	$R$ ( $\text{\AA}$ )	$\Theta_{\text{cD}}$ (K)	$\sigma_{\text{stat}}^2$ ( $\text{\AA}^2$ )
Mo-O(1)	0.0045(3)	2.030(2)	950(40)	0.0024(1)
Mo-Mo	0.035(1)	3.628(2)*	260( <i>fixed</i> )	0.026(5)
Mo-Y	0.0055(1)	3.628(2)*	356(20)	0.0033(4)
Y-O(1)	0.0092(3)	2.441(1)	525(12)	0.0046(3)
Y-O(2)	0.0036(1)	2.225(1)	860(60)	0.0009(3)
Y-Y/Mo	0.0042(1)	3.609(1)	381(1)	0.0020(2)

# FIGURES

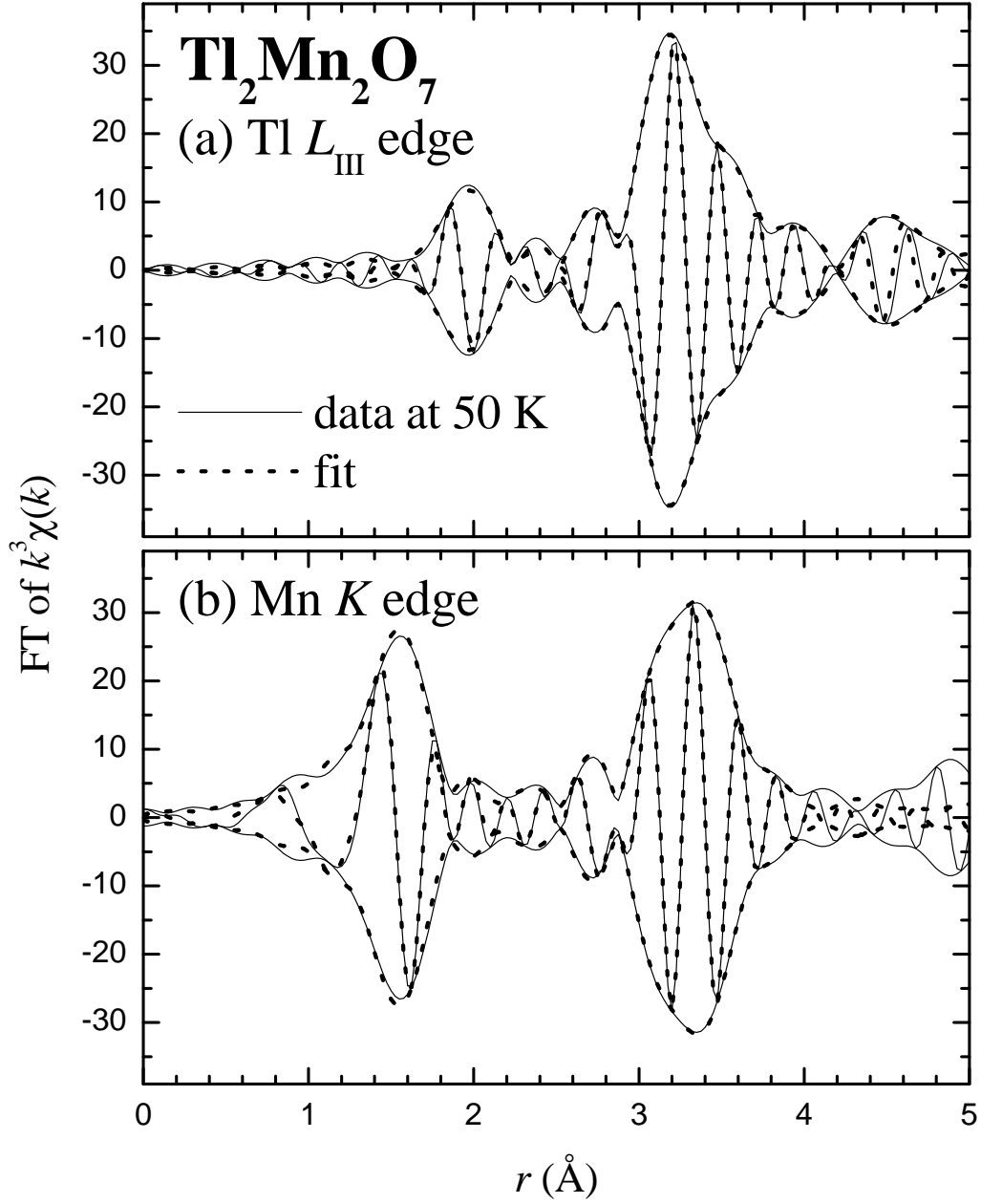


FIG. 1. XAFS data and fits on  $\text{Tl}_2\text{Mn}_2\text{O}_7$ . The outer envelope shows  $\pm$  the amplitude (or modulus) and the oscillating inner curve is the real part of each complex transform. The  $r$ -axis includes different phase shifts for each coordination shell, so that the  $r$  of a given peak does not equal the pair distance  $R$ . Transforms are from 3.0 and 15.0  $\text{\AA}^{-1}$ , and Gaussian narrowed by 0.3  $\text{\AA}^{-1}$ . Fits are from 1.0 and 4.0  $\text{\AA}$ .



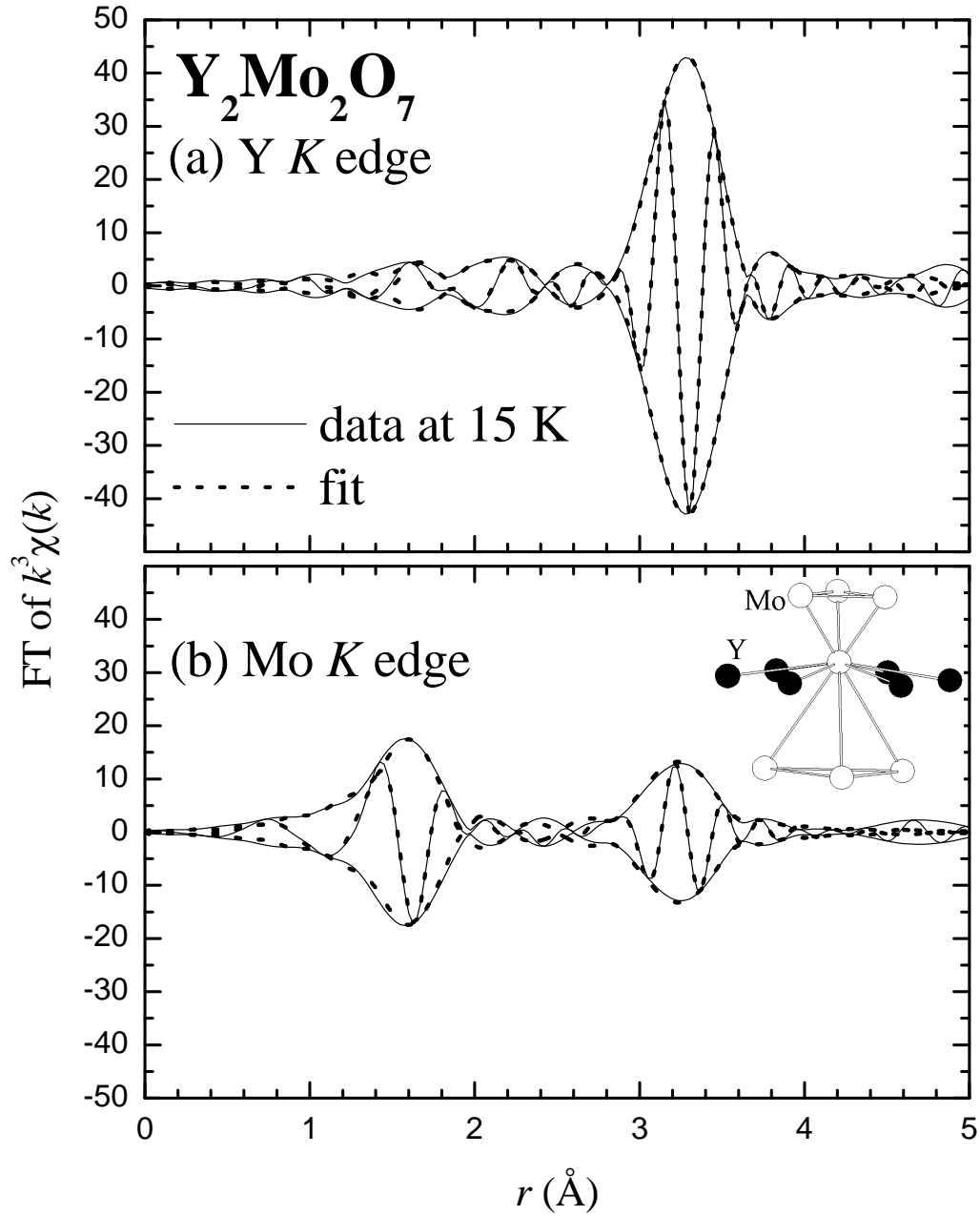


FIG. 2. XAFS data and fits on Y<sub>2</sub>Mo<sub>2</sub>O<sub>7</sub>. Fit and transform ranges are as in Fig. 1. The inset shows one possible (exaggerated) distortion of the Mo tetrahedra that might explain the difference in the peak amplitude at 3.3 Å between the two edges. Oxygens are omitted for clarity.